Supporting Information for "Heterolytic Benzene C-H Activation by a Cyclometallated Iridium(III) Bishydroxo Pyridyl Complex: Synthesis, Hydrogen-Deuterium Exchange, and Density Functional Study"

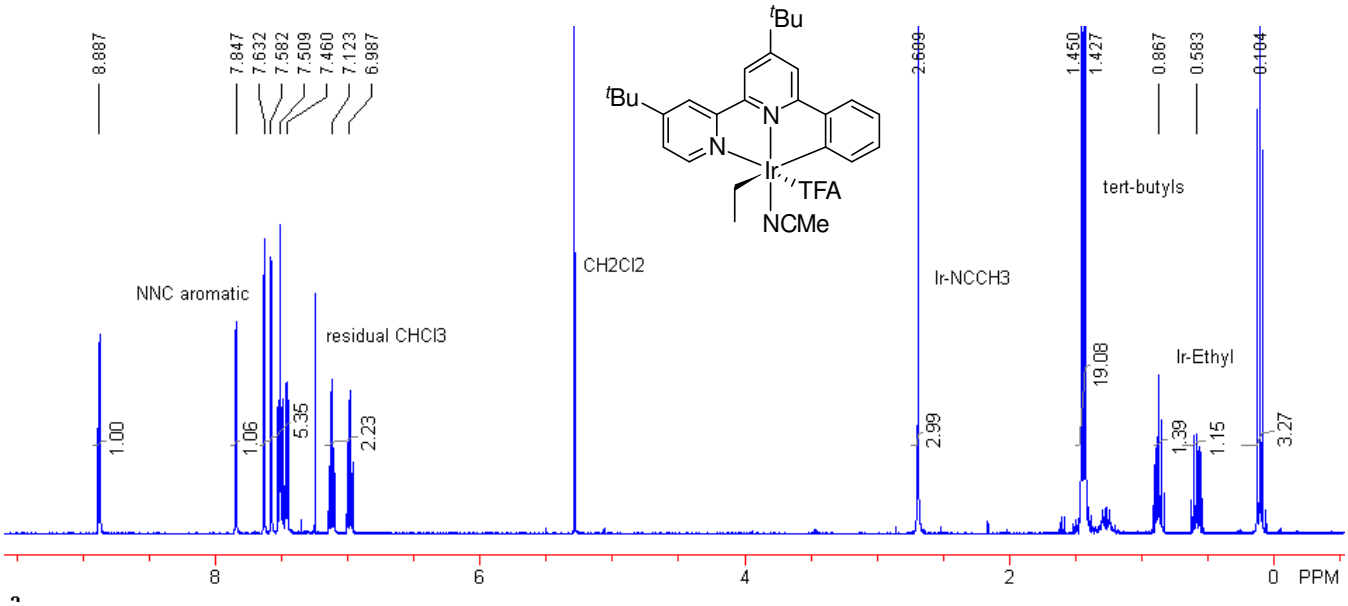

Figure S1. Proton NMR of **2** in $CDCl_3$.

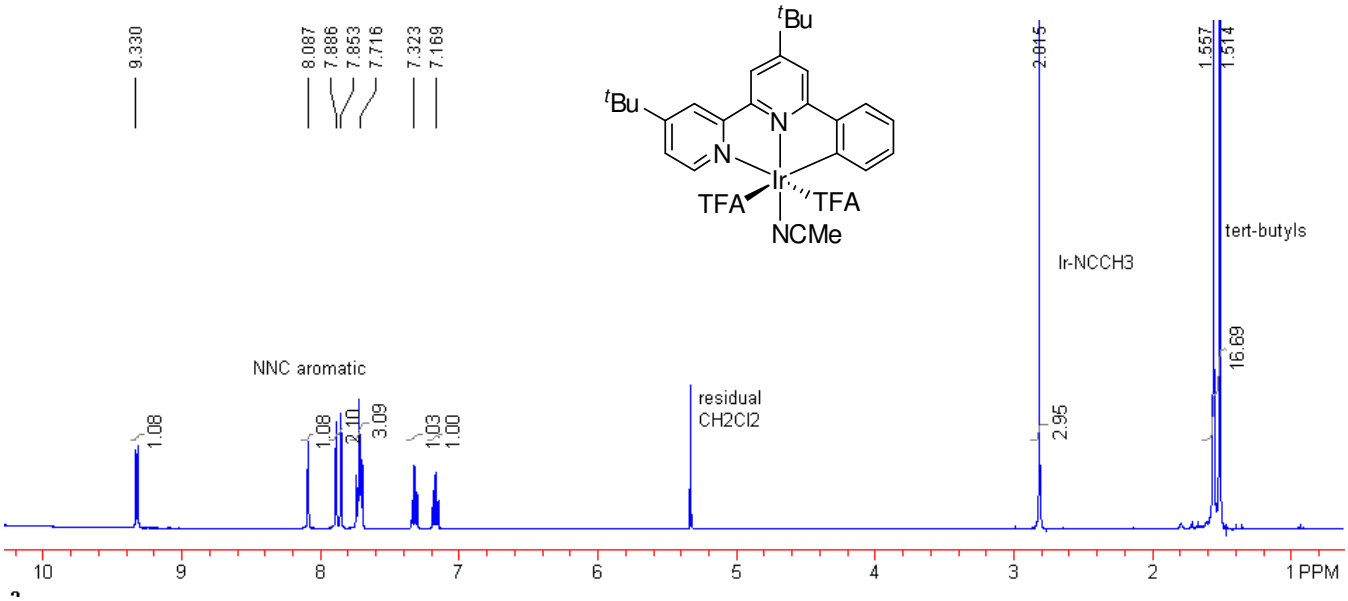

Figure S2. Proton NMR of **3** in CD_2Cl_2.

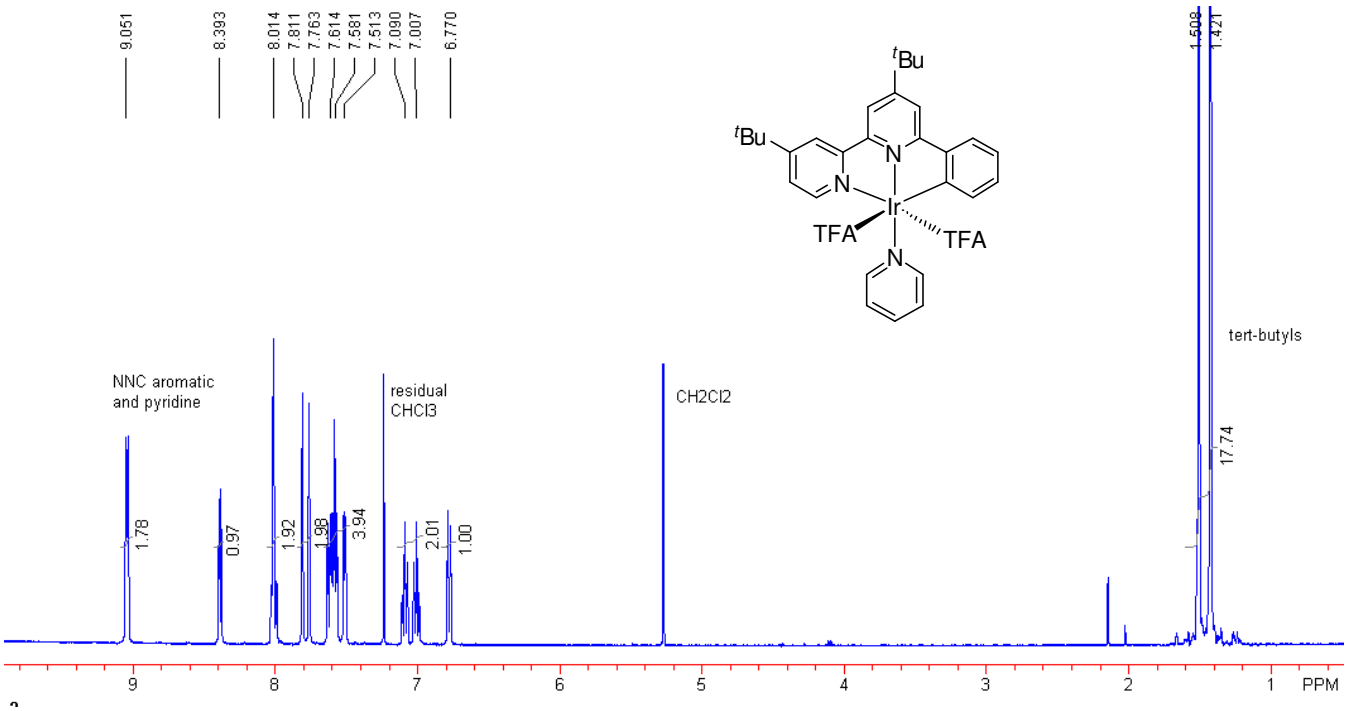

Figure S3. Proton NMR of **4** in $CDCl_3$.

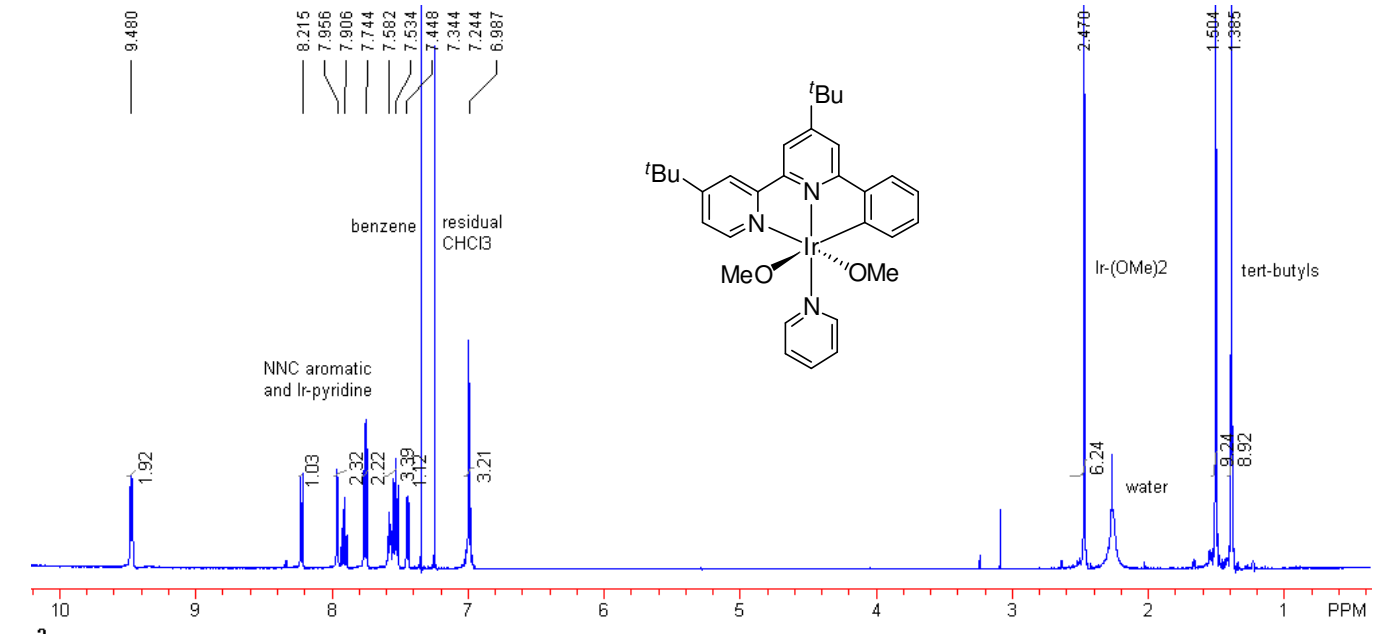

Figure S4. Proton NMR of **5** in $CDCl_3$.

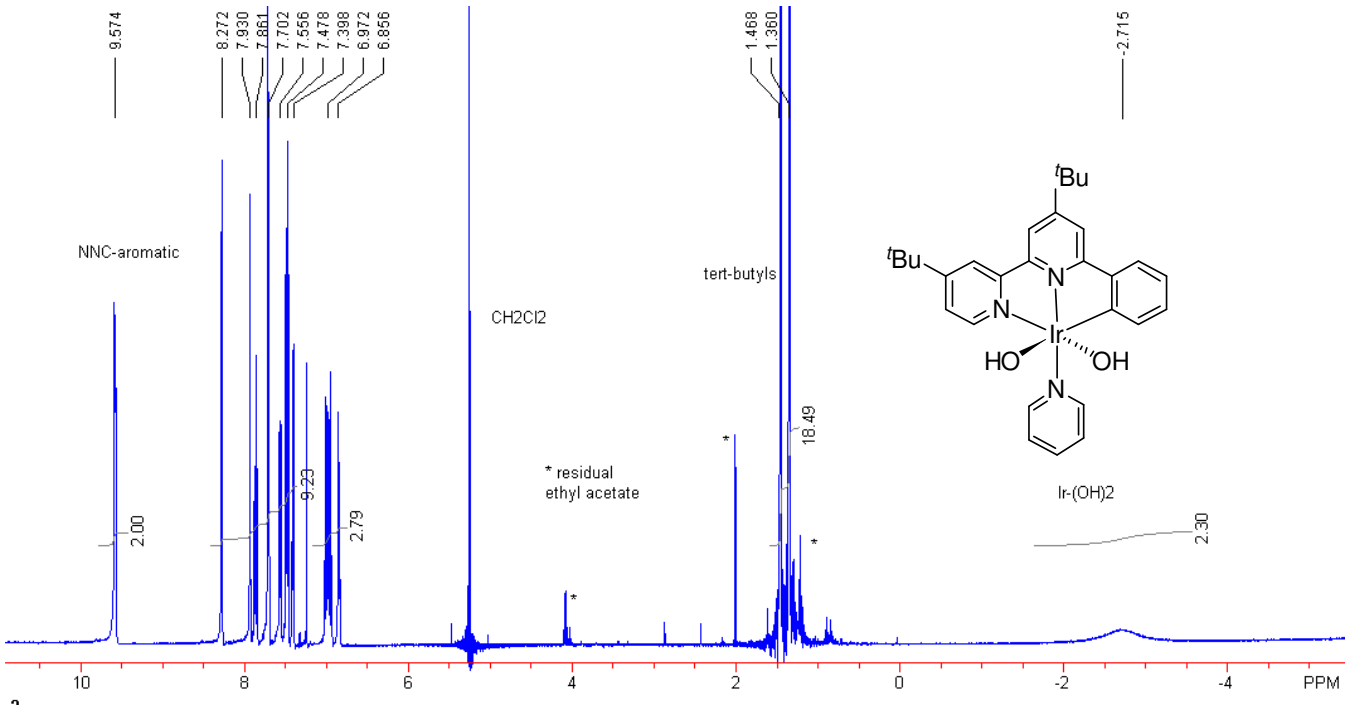

Figure S5. Proton NMR of **6** in $CDCl_3$.

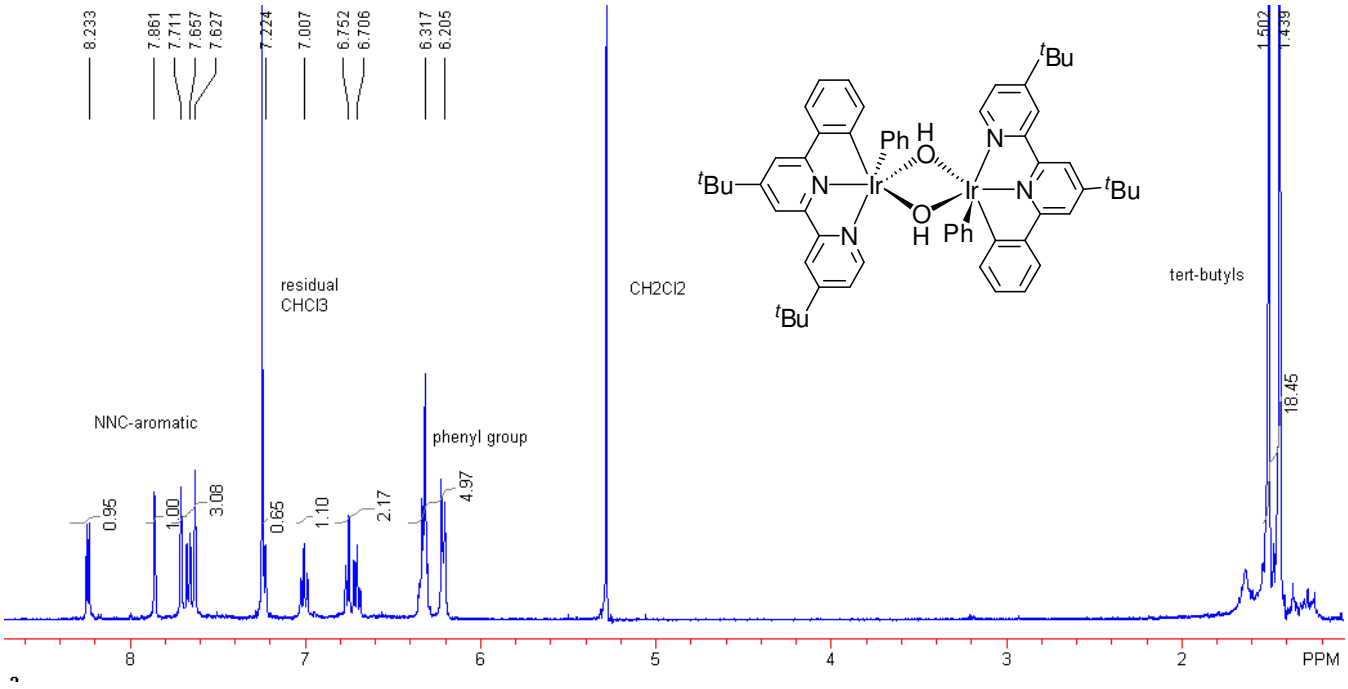

Figure S6. Proton NMR of **9** in $CDCl_3$.

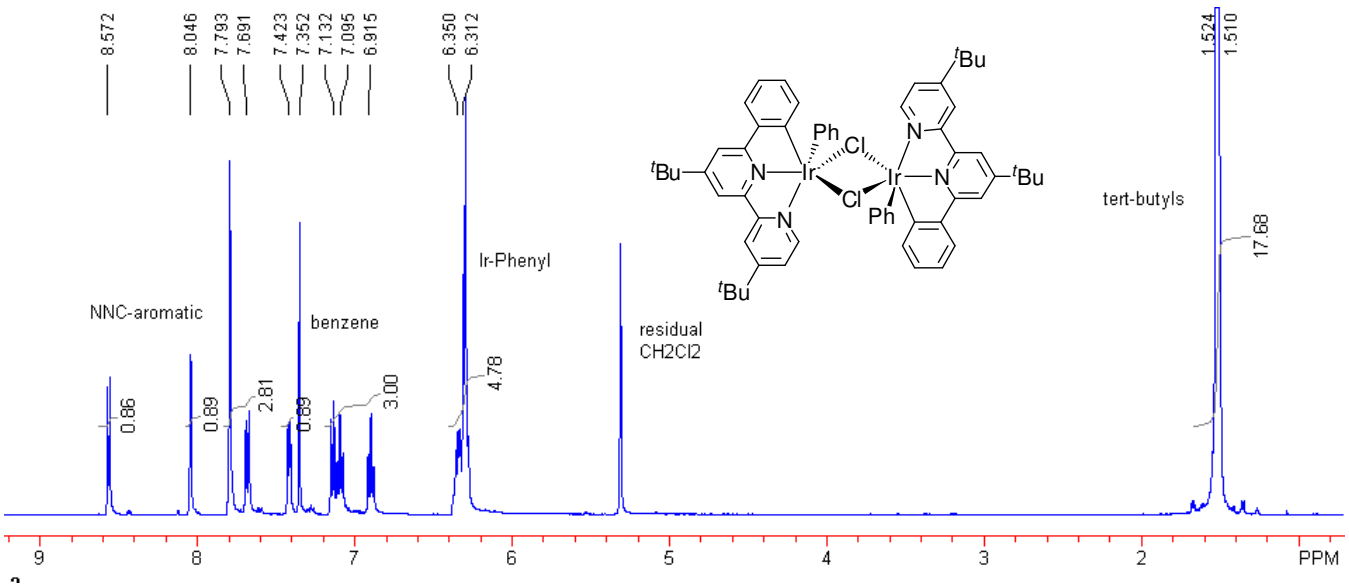

Figure S7. Proton NMR of **10** in CD_2Cl_2**.**

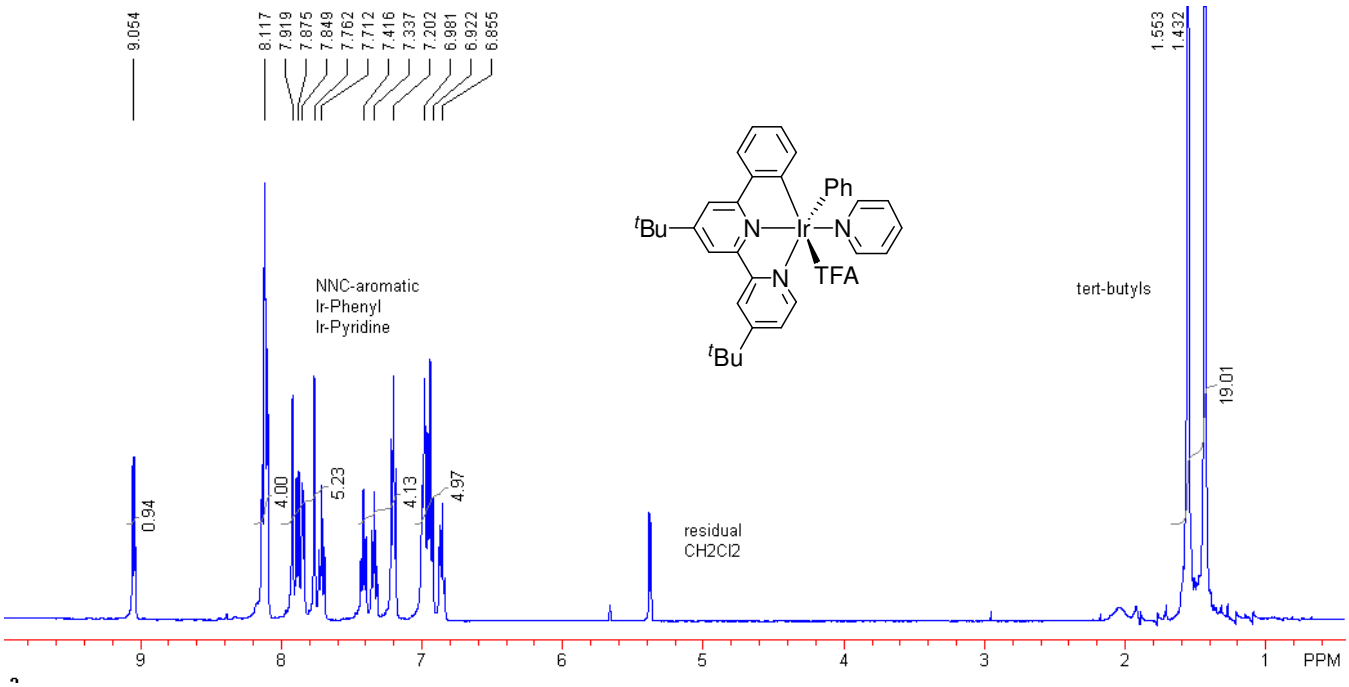

Figure S8. Proton NMR of **11** in CD_2Cl_2.

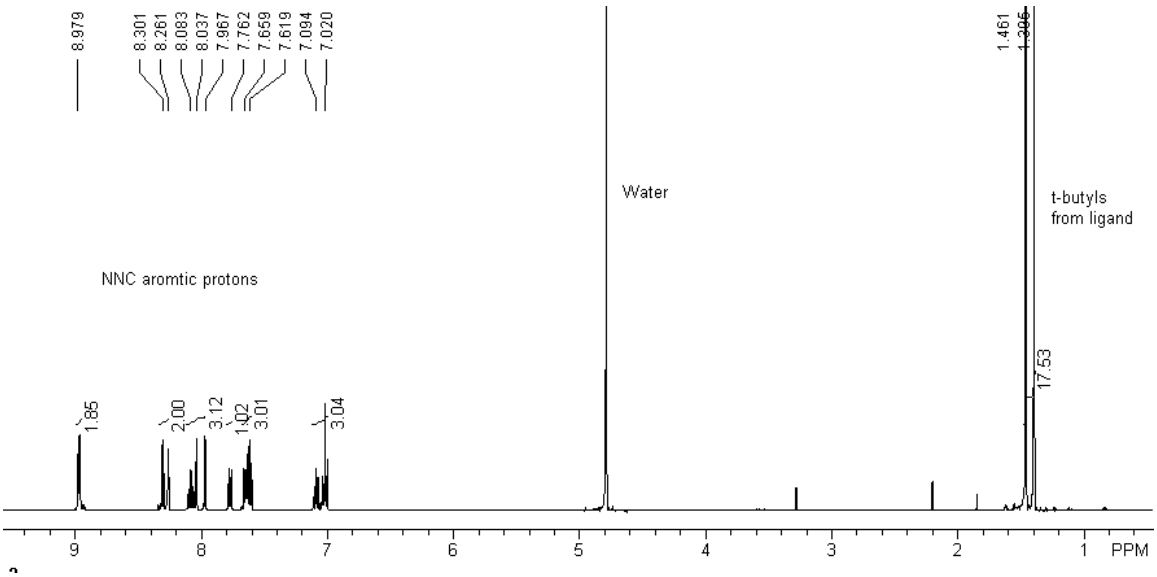

Figure S9. Proton NMR of a 5.0 mM solution of **6** in D_2O.

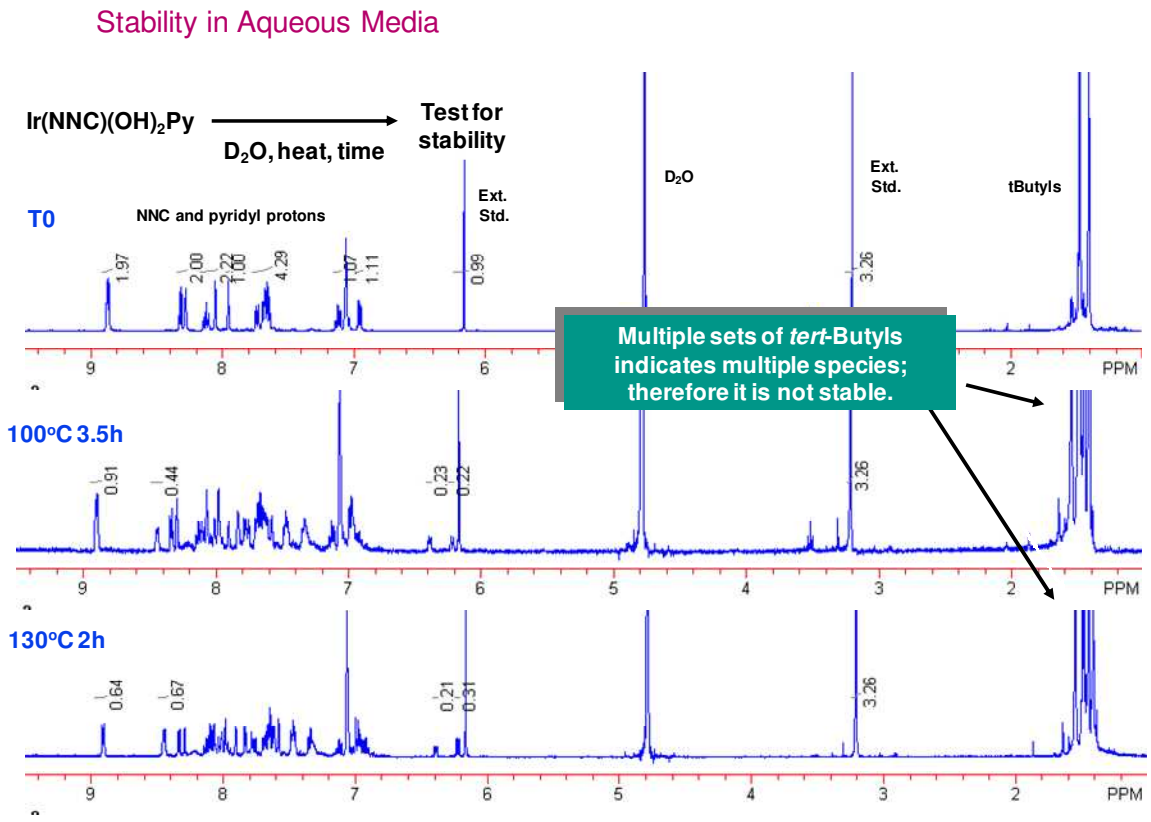

Figure S10. Stability of **6** in D_2O over time.

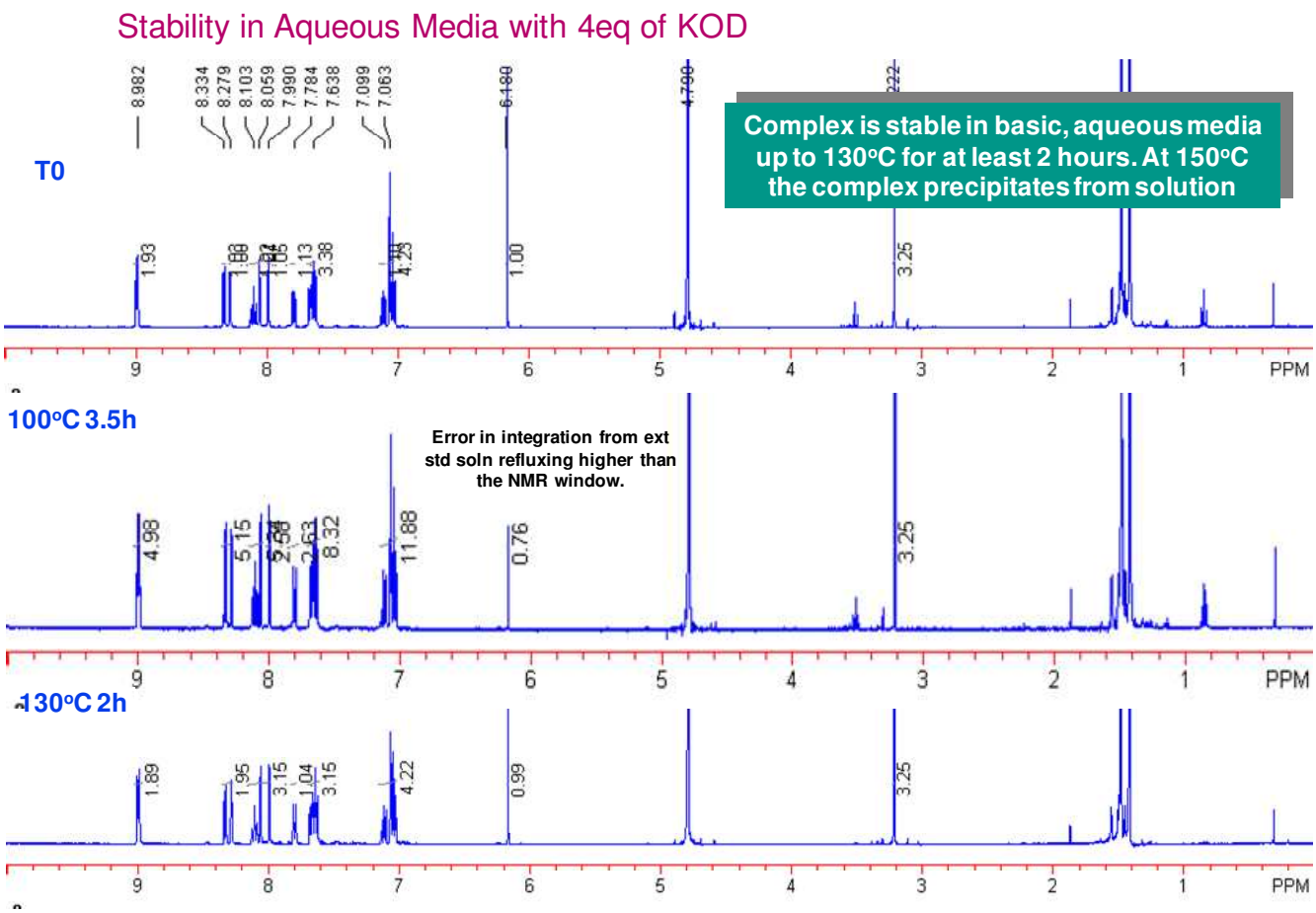

Figure S11. Stability of **6** in D_2O over time in the presence of 4 eq of KOD.

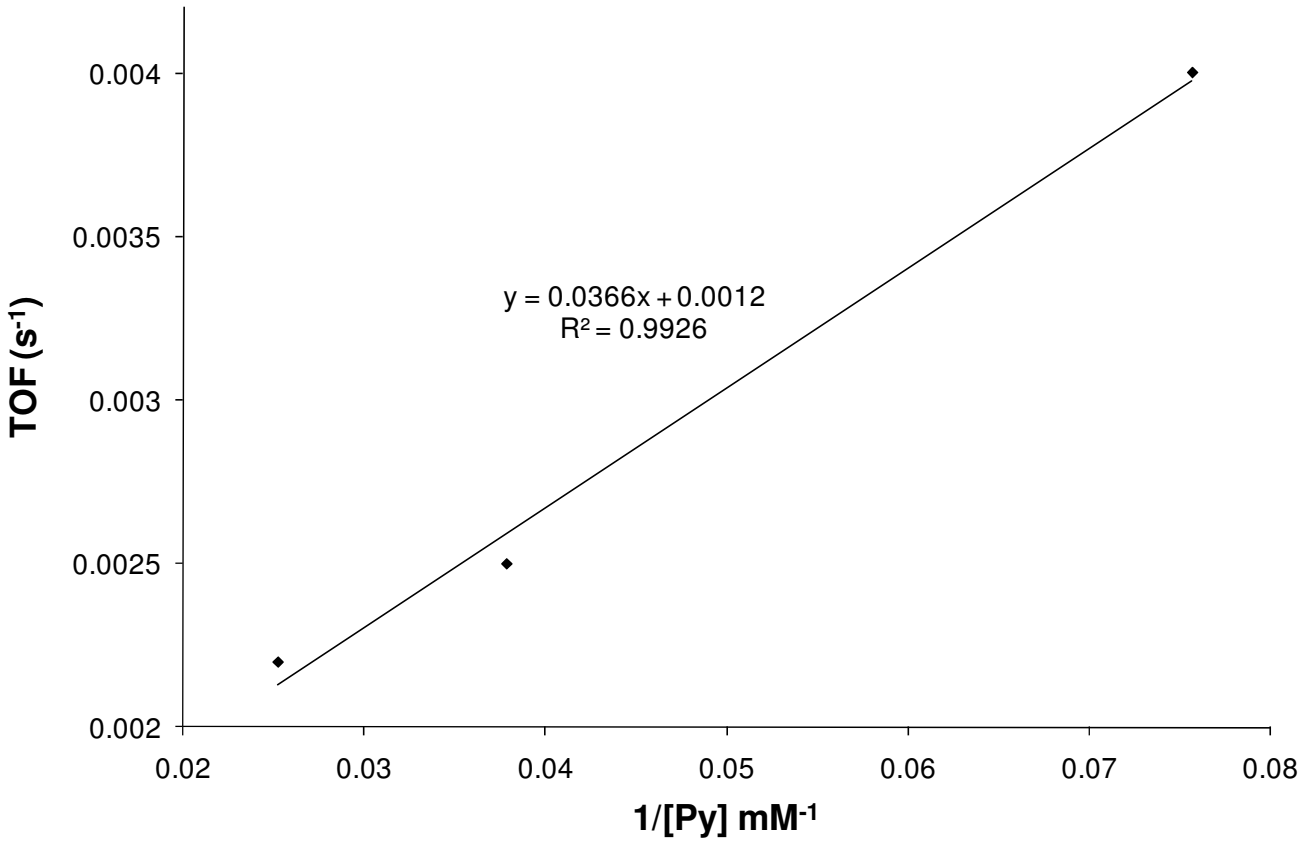

Figure S 12. 1/[Py] Plot for water and benzene H/D exchange using 6 as a catalyst.

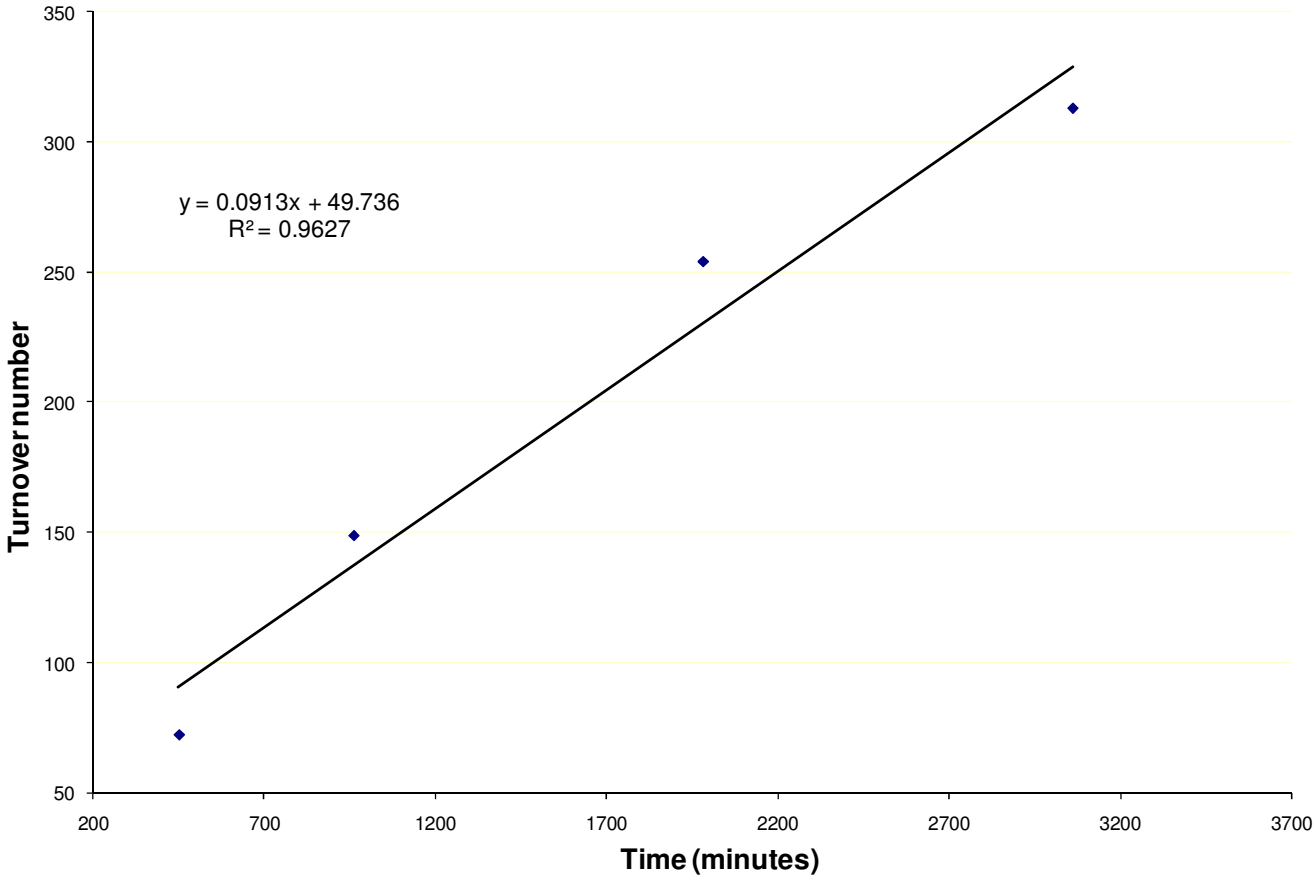

Figure S13. Plot of TON vs. time for a 2.13 mM solution of **6** in 0.5 mL benzene-H_6 and 0.5 mL D_2O with 78 eq (0.16 M) KOD at 180 ^oC.

X-ray structure determination of [(NNC$^{(t\text{-Bu})}$)IrPh(μ-OH)]$_2$ (9)). Suitable black crystals of **9** for X-ray analysis were grown from a CH_2Cl_2 / pentane mixture at –20 ^oC. Diffraction data was collected at 138 K with graphite-monochromatic Mo Kα radiation (λ = 0.71073 Å). The cell parameters were obtained from the least-squares refinement of the spots (collected 60 frames) using the SMART program. A hemisphere of data was collected and the intensity data was processed using the Saint Plus program. All calculations for the structure determination were carried out using the SHELXTL package (version 5.1).[1] Initial atomic positions were located by direct methods using XS, and the structure was refined by least-squares methods using SHELX. Absorption corrections were applied by using SADABS.[2] Calculated hydrogen positions were input and refined in a riding manner along with the attached carbons. The thermal ellipsoid plots are shown in Figure S14 and Figure S15. There are 2 molecules in the unit cell, and it co-crystallized with a CH_2Cl_2 (solvent) molecule and a molecule of

water. Crystal data and refinement parameters can be found in Table S1. Selected bond lengths and angles can be found in Table S3 and Table S4.

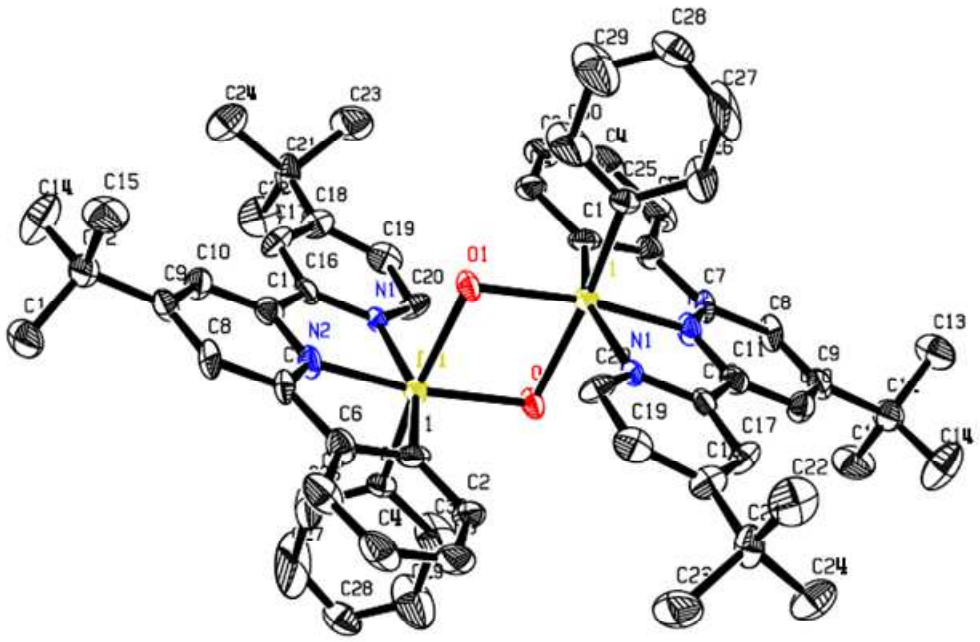

Figure S14. ORTEP of **9**. (Thermal ellipsoids at 50 % probability, and a molecule of water and CH_2Cl_2 omitted for clarity).

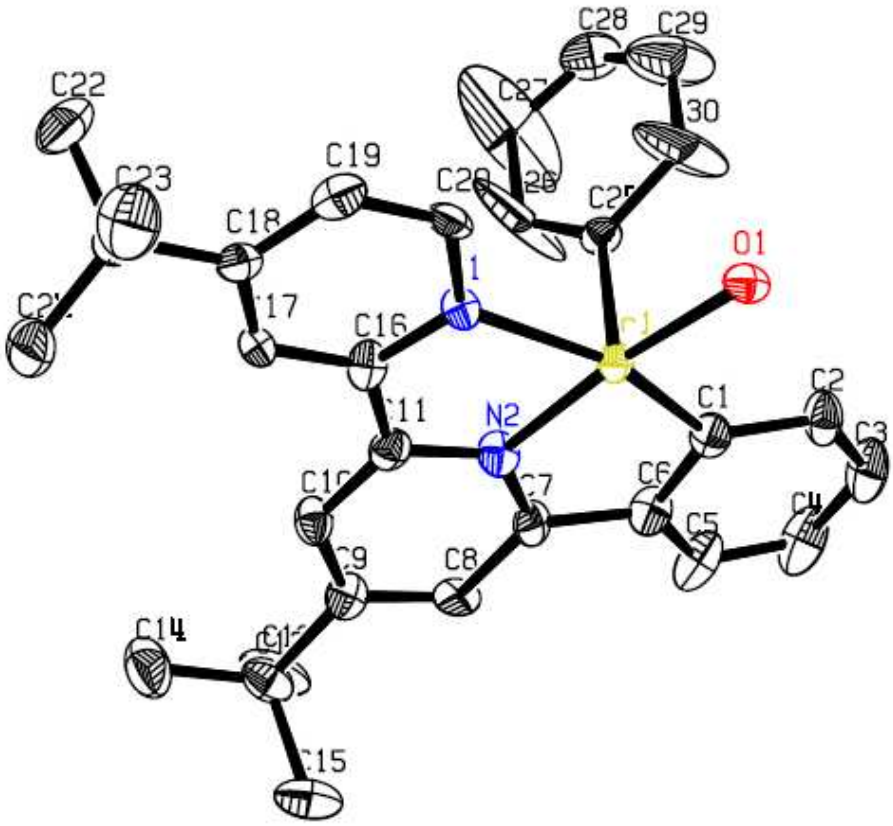

Figure S15. ORTEP of **9** asymmetric unit for clarity of atom naming. (Thermal ellipsoids at 50 % probability, and a molecule of water and CH_2Cl_2 omitted for clarity).

Table S1. Crystal data and structure refinement for $C_{60}H_{66}Ir_2N_4O_2$.

Identification code	irackx2m
Empirical formula	$C_{60}H_{66}Ir_2N_4O_2$
Formula weight	1459.40
Temperature	138(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.009(2) Å α= 88.518(3)°.
	b = 12.096(3) Å β= 88.768(4)°.
	c = 12.500(3) Å γ = 81.758(4)°.
Volume	1497.0(6) $Å^3$
Z	1
Density (calculated)	1.619 Mg/m^3
Absorption coefficient	4.668 mm^{-1}
F(000)	722
Crystal size	0.30 x 0.15 x 0.20 mm^3
Theta range for data collection	1.63 to 27.54°.
Index ranges	-11<=h<=13, -15<=k<=15, -14<=l<=16
Reflections collected	4975
Independent reflections	3378 [R(int) = 0.0321]
Completeness to theta = 27.54°	49.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3378 / 0 / 344
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0545, wR2 = 0.1534
R indices (all data)	R1 = 0.0569, wR2 = 0.1562
Largest diff. peak and hole	3.265 and -0.921 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for $C_{60}H_{66}Ir_2N_4O_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	9965(1)	9670(1)	1295(1)	21(1)
N(1)	10978(9)	7988(8)	1144(7)	19(2)
N(2)	8756(11)	8819(9)	2129(8)	25(2)
O(1)	11073(8)	10522(7)	192(6)	24(2)
O(2)	5371(9)	8763(7)	-28(7)	29(2)
Cl(1)	1461(8)	6664(7)	4626(8)	102(2)
Cl(2)	-829(11)	6235(8)	5895(7)	116(3)
C(1)	8659(14)	10949(10)	1819(11)	28(3)
C(2)	8670(16)	12126(10)	1722(11)	33(3)
C(3)	7711(18)	12871(11)	2176(12)	41(3)
C(4)	6666(19)	12502(13)	2806(13)	46(4)
C(5)	6596(17)	11386(13)	2925(12)	40(3)
C(6)	7577(14)	10609(11)	2427(11)	30(3)
C(7)	7639(14)	9373(11)	2534(10)	26(2)
C(8)	6655(11)	8786(11)	3021(10)	26(2)
C(9)	6902(13)	7616(10)	3066(10)	27(2)
C(10)	8117(13)	7086(10)	2626(10)	27(2)
C(11)	9032(12)	7686(10)	2149(10)	25(2)
C(12)	5783(15)	6972(12)	3553(11)	34(3)
C(13)	5341(16)	7387(17)	4671(12)	49(4)
C(14)	6193(19)	5722(14)	3639(19)	55(5)
C(15)	4530(15)	7233(16)	2779(13)	48(4)
C(16)	10301(13)	7233(10)	1629(9)	24(2)
C(17)	10766(13)	6096(10)	1549(12)	29(3)
C(18)	11977(12)	5712(10)	988(12)	29(3)
C(19)	12695(14)	6521(11)	560(12)	33(3)
C(20)	12190(12)	7653(10)	660(11)	28(3)
C(21)	12493(13)	4492(11)	874(11)	32(3)
C(22)	13637(17)	4147(15)	1651(16)	50(4)
C(23)	13060(20)	4290(14)	-317(15)	53(4)
C(24)	11356(16)	3765(12)	1062(15)	45(4)
C(25)	11087(12)	9918(9)	2545(9)	22(2)
C(26)	11120(30)	9390(30)	3506(16)	120(14)
C(27)	12050(50)	9510(40)	4290(20)	200(30)
C(28)	12806(15)	10343(14)	4274(13)	41(3)
C(29)	12880(20)	10850(30)	3330(16)	80(8)
C(30)	12030(20)	10670(30)	2448(16)	87(10)
C(31)	140(30)	7220(20)	5445(19)	78(7)

Table S3. Bond lengths [Å] for $C_{60}H_{66}Ir_2N_4O_2$.

Ir(1)-N(2)	1.964(10)
Ir(1)-C(1)	1.991(14)
Ir(1)-C(25)	1.997(11)
Ir(1)-O(1)	2.093(8)
Ir(1)-N(1)	2.150(9)
Ir(1)-O(1)#1	2.182(8)
N(1)-C(16)	1.338(15)
N(1)-C(20)	1.358(15)
N(2)-C(7)	1.316(18)
N(2)-C(11)	1.358(16)
O(1)-Ir(1)#1	2.182(8)
Cl(1)-C(31)	1.72(2)
Cl(2)-C(31)	1.72(3)
C(1)-C(6)	1.413(19)
C(1)-C(2)	1.427(16)
C(2)-C(3)	1.35(2)
C(3)-C(4)	1.41(2)
C(4)-C(5)	1.37(2)
C(5)-C(6)	1.405(19)
C(6)-C(7)	1.491(18)
C(7)-C(8)	1.413(15)
C(8)-C(9)	1.402(18)
C(9)-C(10)	1.399(18)
C(9)-C(12)	1.558(17)
C(10)-C(11)	1.367(17)
C(11)-C(16)	1.456(18)
C(12)-C(14)	1.51(2)
C(12)-C(13)	1.532(18)
C(12)-C(15)	1.59(2)
C(16)-C(17)	1.393(17)
C(17)-C(18)	1.413(19)
C(18)-C(19)	1.385(19)
C(18)-C(21)	1.501(18)
C(19)-C(20)	1.398(18)
C(21)-C(22)	1.52(2)
C(21)-C(24)	1.546(18)
C(21)-C(23)	1.59(2)
C(25)-C(26)	1.34(2)
C(25)-C(30)	1.41(2)
C(26)-C(27)	1.40(3)
C(27)-C(28)	1.34(3)
C(28)-C(29)	1.32(3)
C(29)-C(30)	1.44(2)

Table S4. Bond angles [°] for $C_{60}H_{66}Ir_2N_4O_2$.

Atom-Atom-Atom	Degrees	Atom-Atom-Atom	Degrees
N(2)-Ir(1)-C(1)	81.6(5)	N(2)-Ir(1)-C(25)	94.5(5)
C(1)-Ir(1)-C(25)	86.4(5)	N(2)-Ir(1)-O(1)	170.7(4)
C(1)-Ir(1)-O(1)	99.5(5)	C(25)-Ir(1)-O(1)	94.8(4)
N(2)-Ir(1)-N(1)	78.3(4)	C(1)-Ir(1)-N(1)	159.6(5)
C(25)-Ir(1)-N(1)	91.4(4)	O(1)-Ir(1)-N(1)	100.9(3)
N(2)-Ir(1)-O(1)#1	92.4(4)	C(1)-Ir(1)-O(1)#1	95.9(4)
C(25)-Ir(1)-O(1)#1	173.0(4)	O(1)-Ir(1)-O(1)#1	78.3(3)
N(1)-Ir(1)-O(1)#1	88.7(3)	C(16)-N(1)-C(20)	119.9(10)
C(16)-N(1)-Ir(1)	112.7(8)	C(20)-N(1)-Ir(1)	127.4(7)
C(7)-N(2)-C(11)	123.4(11)	C(7)-N(2)-Ir(1)	117.8(8)
C(11)-N(2)-Ir(1)	118.4(9)	Ir(1)-O(1)-Ir(1)#1	101.7(3)
C(6)-C(1)-C(2)	115.9(14)	C(6)-C(1)-Ir(1)	113.0(9)
C(2)-C(1)-Ir(1)	131.1(12)	C(3)-C(2)-C(1)	122.4(15)
C(2)-C(3)-C(4)	120.2(13)	C(5)-C(4)-C(3)	120.1(14)
C(4)-C(5)-C(6)	119.6(16)	C(5)-C(6)-C(1)	121.7(13)
C(5)-C(6)-C(7)	124.5(13)	C(1)-C(6)-C(7)	113.7(12)
N(2)-C(7)-C(8)	120.0(11)	N(2)-C(7)-C(6)	113.4(11)
C(8)-C(7)-C(6)	126.7(13)	C(9)-C(8)-C(7)	118.6(12)
C(10)-C(9)-C(8)	118.1(11)	C(10)-C(9)-C(12)	123.4(11)
C(8)-C(9)-C(12)	118.4(12)	C(11)-C(10)-C(9)	121.3(11)
N(2)-C(11)-C(10)	118.6(12)	N(2)-C(11)-C(16)	115.0(11)
C(10)-C(11)-C(16)	126.4(11)	C(14)-C(12)-C(13)	107.8(15)
C(14)-C(12)-C(9)	114.0(13)	C(13)-C(12)-C(9)	111.3(10)
C(14)-C(12)-C(15)	108.9(13)	C(13)-C(12)-C(15)	108.6(13)
C(9)-C(12)-C(15)	106.2(12)	N(1)-C(16)-C(17)	120.4(11)
N(1)-C(16)-C(11)	115.3(10)	C(17)-C(16)-C(11)	124.1(11)
C(16)-C(17)-C(18)	121.2(11)	C(19)-C(18)-C(17)	116.7(11)
C(19)-C(18)-C(21)	120.9(12)	C(17)-C(18)-C(21)	122.5(11)
C(18)-C(19)-C(20)	120.1(13)	N(1)-C(20)-C(19)	121.4(11)
C(18)-C(21)-C(22)	109.7(12)	C(18)-C(21)-C(24)	111.5(10)
C(22)-C(21)-C(24)	110.6(13)	C(18)-C(21)-C(23)	108.7(12)
C(22)-C(21)-C(23)	108.9(13)	C(24)-C(21)-C(23)	107.4(12)
C(26)-C(25)-C(30)	112.5(13)	C(26)-C(25)-Ir(1)	127.5(9)
C(30)-C(25)-Ir(1)	119.9(11)	C(25)-C(26)-C(27)	123.9(16)
C(28)-C(27)-C(26)	123(2)	C(29)-C(28)-C(27)	114.2(18)
C(28)-C(29)-C(30)	123(2)	C(25)-C(30)-C(29)	121.0(19)
Cl(2)-C(31)-Cl(1)	112.5(14)		

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+2,-z

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{60}H_{66}Ir_2N_4O_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	23(1)	21(1)	18(1)	1(1)	0(1)	-3(1)
N(1)	22(4)	21(4)	13(4)	-3(3)	8(3)	-4(4)
N(2)	26(5)	28(5)	20(5)	1(4)	11(4)	-3(4)
O(1)	21(4)	36(4)	16(4)	4(3)	1(3)	-8(3)
Cl(1)	78(4)	103(5)	128(7)	-23(5)	17(4)	-19(4)
Cl(2)	147(8)	116(6)	95(5)	-21(5)	49(5)	-58(6)
C(1)	37(7)	22(5)	25(6)	-5(5)	-11(5)	-6(5)
C(2)	54(8)	20(5)	27(7)	-2(5)	-9(6)	-8(5)
C(3)	68(10)	18(5)	34(7)	-8(5)	-3(7)	4(6)
C(4)	69(11)	34(7)	28(7)	-6(6)	6(7)	19(7)
C(5)	52(9)	37(7)	26(7)	-1(6)	-1(6)	15(6)
C(6)	32(6)	30(6)	25(6)	1(5)	7(5)	2(5)
C(7)	32(6)	28(6)	19(6)	10(5)	1(5)	-6(5)
C(8)	13(5)	41(6)	24(6)	6(5)	13(4)	-5(5)
C(9)	33(6)	30(6)	17(6)	3(5)	2(5)	-3(5)
C(10)	31(6)	20(5)	29(6)	-1(5)	8(5)	-2(5)
C(11)	28(6)	27(5)	21(6)	1(5)	-5(4)	-2(5)
C(12)	34(7)	42(7)	28(7)	-2(6)	4(5)	-16(6)
C(13)	38(8)	83(12)	32(8)	-13(8)	14(6)	-34(9)
C(14)	40(9)	33(8)	91(15)	4(8)	21(9)	-8(7)
C(15)	34(8)	70(10)	45(9)	-10(8)	-9(6)	-18(8)
C(16)	35(6)	23(5)	12(5)	0(4)	2(4)	-2(5)
C(17)	25(6)	20(5)	43(8)	4(5)	-7(5)	-8(4)
C(18)	21(6)	27(6)	39(7)	-1(5)	-6(5)	-2(5)
C(19)	28(6)	38(7)	33(7)	-3(6)	-6(5)	2(5)
C(20)	19(5)	24(5)	42(7)	-5(5)	-2(5)	-9(4)
C(21)	25(6)	32(6)	36(7)	6(5)	16(5)	3(5)
C(22)	38(8)	41(8)	66(11)	2(8)	-11(7)	12(7)
C(23)	66(11)	38(8)	53(11)	-18(8)	5(8)	1(8)
C(24)	39(8)	25(6)	69(11)	-7(7)	5(7)	1(6)
C(25)	23(5)	24(5)	20(5)	-4(4)	-5(4)	-3(4)
C(26)	170(30)	190(30)	42(11)	42(14)	-44(13)	-170(30)
C(27)	340(60)	280(50)	51(15)	100(20)	-120(30)	-250(50)
C(28)	37(7)	58(9)	29(7)	-7(7)	-7(5)	-4(7)
C(29)	53(11)	150(20)	44(11)	15(13)	-16(8)	-44(15)
C(30)	76(14)	170(30)	39(10)	8(13)	-23(9)	-90(18)
C(31)	85(16)	80(15)	65(14)	-17(12)	-15(12)	3(13)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_{60}H_{66}Ir_2N_4O_2$.

	x	y	z	U(eq)
H(2)	9380	12393	1322	40
H(3)	7737	13649	2073	49
H(4)	6011	13030	3148	56
H(5)	5888	11136	3342	48
H(8)	5843	9177	3311	32
H(10)	8308	6294	2660	32
H(13A)	4551	7050	4913	73
H(13B)	5110	8202	4644	73
H(13C)	6081	7174	5170	73
H(14A)	6988	5554	4091	82
H(14B)	6409	5425	2924	82
H(14C)	5447	5375	3959	82
H(15A)	4843	7139	2035	72
H(15B)	4093	8003	2877	72
H(15C)	3881	6717	2950	72
H(17)	10259	5569	1878	34
H(19)	13532	6306	197	40
H(20)	12707	8200	385	33
H(22A)	14433	4480	1414	75
H(22B)	13859	3331	1672	75
H(22C)	13354	4409	2368	75
H(23A)	12460	4748	-818	80
H(23B)	13090	3499	-484	80
H(23C)	13967	4497	-381	80
H(24A)	11140	3723	1830	67
H(24B)	11656	3012	801	67
H(24C)	10550	4100	676	67
H(26)	10466	8908	3659	144
H(27)	12151	8985	4872	245
H(28)	13253	10548	4885	50
H(29)	13518	11351	3227	96
H(30)	12114	11074	1792	105
H(31A)	511	7557	6068	94
H(31B)	-431	7819	5048	94

B3LYP/LACVP** Transition State Coordinates

TS1

N1	-0.0037235147	0.0080228775	-0.0012111515
C2	-0.0046946964	0.0546075538	2.7430837703
C3	1.1863827648	0.0227195947	0.6550517092
C4	-1.2032658588	-0.0517742004	0.6489964726
C5	-1.2096354996	-0.0158593179	2.0461764906
C6	1.2055002222	0.0643673145	2.0502081688
H7	-2.1518192910	-0.0496525208	2.5812156057
H8	2.1459575798	0.0959962955	2.5876311979
N9	2.1161804437	-0.0228495251	-1.5616286742
C10	4.7360904757	-0.1674096114	-0.6691185275
C11	3.1225982925	-0.1197877167	-2.4393900201
C12	2.3722053615	-0.0232318314	-0.2251171715
C13	3.6888057020	-0.0876427988	0.2430044862
C14	4.4522073838	-0.1905167261	-2.0353726482
H15	3.8906502226	-0.0861896302	1.3080638236
H16	5.2413025867	-0.2647650707	-2.7757643863
C17	-2.0100694136	-0.1798258539	-1.6616496408
C18	-4.7031657971	-0.3603752975	-0.7615969611
C19	-2.3416330356	-0.1587485875	-0.2679127597
C20	-3.0765160696	-0.3059536587	-2.5641852206
C21	-4.4006777471	-0.3940080421	-2.1268057380
C22	-3.6727494181	-0.2440314466	0.1667048689
H23	-5.2037882704	-0.4892792962	-2.8540738848

H24	-3.9100952175	-0.2230241868	1.2276852670
H25	-5.7342473153	-0.4277273830	-0.4268659497
Ir26	-0.0142702483	-0.0419836094	-1.9603003469
H27	2.8227763262	-0.1379183513	-3.4830714603
H28	-2.8756860741	-0.3285548226	-3.6335641175
O29	0.2358795606	-2.0494691940	-1.9017904244
H30	-0.6459321525	-2.4449329272	-1.9109819932
O31	0.1353616651	0.1773847357	-4.0845277245
H32	-0.6801475518	-0.1315303655	-4.5007984500
C33	-0.1133450517	2.2242548695	-2.4440900176
C34	-1.3206045817	2.9173499347	-2.2105275257
C35	-1.3339004338	4.2727449039	-1.8847824063
C36	-0.1328190303	4.9791652172	-1.7907191328
C37	1.0786275515	4.3291130507	-2.0390788215
C38	1.0810735879	2.9739851184	-2.3637911279
H39	-0.0897400071	1.3136032765	-3.4188260554
H40	-2.2615828590	2.3818212649	-2.2864389106
H41	-2.2778288978	4.7807911318	-1.7036684009
H42	-0.1408427329	6.0357897895	-1.5343658388
H43	2.0138971918	4.8806557497	-1.9817296838
H44	2.0290976295	2.4865794914	-2.5740259872
H45	-0.0069026169	0.0872382891	3.8280913538
H46	5.7616460410	-0.2183405382	-0.3162482766

TS2

N1	0.0021454312	-0.0065498642	0.0035785282
C2	0.0007929396	-0.0227981631	2.7461280600

C3	1.1912525260	-0.0144144093	0.6574339771
C4	-1.1965229246	-0.0603135697	0.6508819387
C5	-1.2051214094	-0.0575341290	2.0499663255
C6	1.2117164272	-0.0119460037	2.0528015581
H7	-2.1476261513	-0.0899618937	2.5848579763
H8	2.1519934036	-0.0046448300	2.5912617841
N9	2.1261118710	-0.0224710865	-1.5608793881
C10	4.7412016374	-0.2177627478	-0.6677473025
C11	3.1308239529	-0.1130493209	-2.4382978540
C12	2.3792939430	-0.0496036154	-0.2253347046
C13	3.6928023697	-0.1395943671	0.2446018069
C14	4.4593545175	-0.2111540097	-2.0338014238
H15	3.8932674422	-0.1603258018	1.3097510839
H16	5.2490433283	-0.2845813766	-2.7739310610
C17	-2.0008653944	-0.1655194080	-1.6661927640
C18	-4.6951136092	-0.3870904818	-0.7654544786
C19	-2.3359877695	-0.1461591118	-0.2708723651
C20	-3.0649072049	-0.3464259487	-2.5654754714
C21	-4.3881714161	-0.4504941211	-2.1285523970
C22	-3.6671863229	-0.2443710212	0.1623508283
H23	-5.1867807354	-0.5865835994	-2.8544608982
H24	-3.9061178695	-0.2190626223	1.2229990823
H25	-5.7256041518	-0.4630428831	-0.4309509440
Ir26	-0.0084440151	-0.0080936134	-1.9699216879
H27	2.8275557642	-0.1105537778	-3.4813991005
H28	-2.8532859858	-0.4314111828	-3.6296122205

O29	0.2135231918	-2.0295762950	-2.0730681216
H30	-0.6420379433	-2.4218849564	-1.8529309611
O31	0.1574114952	-0.0801529272	-4.0641151655
H32	-0.0559413633	-1.0046823797	-4.2566752645
C33	0.0108660147	2.2719431826	-1.9671236710
C34	-0.7352806800	2.9448230222	-0.9722252721
C35	-0.3002461619	4.1425862130	-0.4074235166
C36	0.8995128631	4.7176091243	-0.8338317839
C37	1.6478337840	4.0999773555	-1.8403643237
C38	1.2021331851	2.9043189896	-2.3976688691
H39	-0.7034055444	1.9343668155	-3.0416432589
H40	-1.6781000347	2.5173004467	-0.6406635936
H41	-0.8943312750	4.6319760314	0.3607050883
H42	1.2424767397	5.6517015884	-0.3953786732
H43	2.5706266483	4.5570937340	-2.1896704285
H44	1.7749662820	2.4458845225	-3.2001081777
O45	-1.2686317117	1.8427752289	-4.2467712134
H46	-0.7134117691	0.8978033852	-4.3701059414
H47	-2.1831274211	1.6017641152	-4.0401951573
H48	0.0000456159	-0.0174947939	3.8318001735
H49	5.7652647159	-0.2924835692	-0.3142448203

TS3

N1	0.0827065167	0.0432729831	0.1133693841
C2	0.1337880577	-0.0083639589	2.8665728971
C3	1.2865862911	0.0331766374	0.7540716832
C4	-1.1080426952	-0.0330948636	0.7906587397

C5	-1.0883329467	-0.0496619091	2.1860676148
C6	1.3302051094	0.0242536541	2.1532457414
H7	-2.0205623085	-0.1041994903	2.7391920584
H8	2.2818112998	0.0300568007	2.6743789471
N9	2.1870039938	0.0043769024	-1.4727119486
C10	4.8163521698	-0.1050968829	-0.6479544261
C11	3.1631053133	-0.0770985814	-2.3817300335
C12	2.4591458216	0.0045077923	-0.1402369351
C13	3.7946672940	-0.0432937519	0.2925493443
C14	4.5027233696	-0.1281868523	-2.0135018564
H15	4.0268393531	-0.0408779172	1.3524675816
H16	5.2796309005	-0.1885342687	-2.7699245675
C17	-1.9462831484	-0.1007489819	-1.5185728058
C18	-4.6319160697	-0.2053442655	-0.5793317164
C19	-2.2565100893	-0.0927972015	-0.1159624284
C20	-3.0297711710	-0.1719352900	-2.4163459972
C21	-4.3443949542	-0.2211977557	-1.9526236406
C22	-3.5870355667	-0.1421467313	0.3351180014
H23	-5.1632233924	-0.2779641914	-2.6692257166
H24	-3.8074220643	-0.1320620461	1.4013227362
H25	-5.6619097556	-0.2458035377	-0.2310451917
Ir26	0.0245387298	-0.0309600449	-1.8872466386
H27	2.7877186809	-0.1015172598	-3.4071362080
H28	-2.8192835821	-0.1843722050	-3.4871216152
O29	0.1405108472	-2.0440920937	-1.7272862855
H30	0.1648261922	-2.2284073650	-2.6818766824

O31	0.3287291258	-0.1430682249	-3.8549718681
H32	-0.8964987737	-0.2216922451	-4.7820904331
C33	0.0524010191	2.3140215224	-2.7178158947
C34	-1.2038955321	2.9458437240	-2.6893423984
C35	-1.3331182239	4.2841090641	-2.3140010061
C36	-0.1993293992	5.0200797910	-1.9610419474
C37	1.0615592101	4.4171795219	-1.9899817982
C38	1.1794340782	3.0789100817	-2.3651849213
H39	0.1973324036	1.3010900294	-3.3898723350
H40	-2.0852096962	2.3697756316	-2.9563902373
H41	-2.3144685453	4.7535096709	-2.2896723885
H42	-0.2970646375	6.0628116102	-1.6648433079
H43	1.9448939189	4.9919545666	-1.7173877841
H44	2.1622829016	2.6155893085	-2.3943734070
H45	0.1503584349	-0.0183411239	3.9530560729
H46	5.8522782890	-0.1446125192	-0.3204733014
O47	-1.7150296903	-0.1393164104	-5.4096102168
H48	-1.7661829318	0.8175638450	-5.5303995073

TS4

N1	-0.0064535090	-0.0226267451	0.0172439315
C2	-0.0019705199	-0.0746484353	2.7649690243
C3	1.1803823785	-0.0239746234	0.6716401067
C4	-1.2029365307	0.0036848324	0.6729987853
C5	-1.2081270726	-0.0295575170	2.0706933198
C6	1.2043864237	-0.0669935639	2.0673022400
H7	-2.1503665310	-0.0157958739	2.6062362871

H8	2.1459828076	-0.0836079820	2.6023761786
N9	2.1263841805	0.0676270618	-1.5406909052
C10	4.7414327630	0.2097852566	-0.5886824959
C11	3.1584521649	0.1912756581	-2.3858287065
C12	2.3678419959	0.0419763320	-0.2016390578
C13	3.6740357352	0.1035739824	0.2951795021
C14	4.4800710683	0.2616669590	-1.9564989349
H15	3.8523509332	0.0803601362	1.3636932764
H16	5.2790218488	0.3603242121	-2.6835000558
C17	-2.0389601895	0.0854407480	-1.6282190973
C18	-4.7286342699	0.0129491289	-0.6970391491
C19	-2.3528671724	0.0475280802	-0.2318139449
C20	-3.1229663796	0.0538699811	-2.5200920584
C21	-4.4442730261	0.0223922468	-2.0657648339
C22	-3.6811738768	0.0187705851	0.2187589419
H23	-5.2595371921	0.0032990094	-2.7854366636
H24	-3.9027137696	-0.0054177572	1.2828253161
H25	-5.7574880472	-0.0084507909	-0.3495471876
Ir26	-0.0441392426	0.0883216886	-1.9598354249
H27	2.9003525357	0.2404952723	-3.4369567167
H28	-2.9372452284	0.0521112907	-3.5904661545
O29	-0.1798081640	-1.9515802995	-2.6605277633
H30	-1.0672942469	-2.2553455724	-2.4213807514
O31	0.1930052344	2.0904485534	-1.7473450091
H32	-0.6884365969	2.4832788572	-1.7875453268
C33	0.0180210984	0.1215235986	-4.2537570394

C34	-0.7035396739	1.2040715972	-4.7930359335
C35	-0.3559174368	1.7668811520	-6.0212794812
C36	0.7032428291	1.2388345840	-6.7633823091
C37	1.4123370066	0.1404490503	-6.2719431359
C38	1.0743278753	-0.4009291365	-5.0316031867
H39	-0.3419835585	-0.9557797488	-3.5691474129
H40	-1.5262653134	1.6351790133	-4.2326323472
H41	-0.9128538796	2.6188881829	-6.4028462050
H42	0.9653821133	1.6725199633	-7.7249376842
H43	2.2212530324	-0.2926845244	-6.8552668423
H44	1.6044548429	-1.2775669376	-4.6653919619
H45	5.7591383152	0.2610007600	-0.2137481827
H46	-0.0000173279	-0.1045268739	3.8501496440

TS5

N1	0.0063799068	0.0135195170	0.0019572480
C2	-0.0308441258	0.0633826519	2.7441733475
C3	1.1951674086	0.0024516490	0.6651507251
C4	-1.1854145919	0.1138397752	0.6375040293
C5	-1.2294974638	0.1258282841	2.0329380061
C6	1.1826663568	0.0120599155	2.0665769147
H7	-2.1758464529	0.1826032415	2.5567948270
H8	2.1174984565	-0.0082150605	2.6142480019
C9	2.0591661694	0.0845884375	-1.6303856751
C10	4.7383505230	0.1219880355	-0.6301981577
C11	3.1659284869	0.2018119496	-2.4856523568
C12	2.3515385050	0.0216142119	-0.2283544844

C13	3.6704498968	0.0299782814	0.2541611818
C14	4.4758240058	0.2176671204	-2.0003195715
H15	3.8658490080	-0.0274825102	1.3222963055
H16	5.3034024521	0.3071367101	-2.7007397905
N17	-2.1248095731	0.0494025396	-1.5828168601
C18	-4.7176212602	0.4947831577	-0.6741665578
C19	-2.3642134514	0.1970865315	-0.2523414015
C20	-3.1490086394	0.1125911665	-2.4444374129
C21	-4.4602649192	0.3369749166	-2.0340359519
C22	-3.6593915487	0.4186383278	0.2253173565
H23	-5.2549340409	0.3846300855	-2.7708196726
H24	-3.8358910728	0.5454123667	1.2868619708
H25	-5.7267048002	0.6750281114	-0.3160815924
Ir26	0.0639755620	0.0176629381	-1.9914893248
H27	3.0072889563	0.2836965228	-3.5544523597
H28	-2.8968690917	-0.0544302094	-3.4843372219
O29	0.1267736205	-2.1422443914	-2.1972210283
H30	-0.2008316610	-2.5403951472	-1.3808375334
O31	-0.1730964701	2.0314406969	-1.8872826177
H32	0.6793494209	2.4228988192	-2.1181121507
C33	0.1789775720	0.1977514811	-4.2551001267
C34	-0.2993066678	1.4344066146	-4.7451238224
C35	0.2179241125	2.0059287823	-5.9064945637
C36	1.2175512830	1.3463144573	-6.6255710694
C37	1.6935518383	0.1077424474	-6.1844933114
C38	1.1772728827	-0.4529323317	-5.0188241235

H39	-0.6863427979	-0.7234919836	-3.9648902107
H40	-1.0488230431	1.9679943273	-4.1696858290
H41	-0.1545055912	2.9669057892	-6.2531921539
H42	1.6187688245	1.7913776065	-7.5329114598
H43	2.4639078697	-0.4115621310	-6.7489873057
H44	1.5372831004	-1.4223552651	-4.6810215828
H45	5.7593893782	0.1298334889	-0.2598927577
H46	-0.0463530082	0.0679025135	3.8299154195
O47	-1.4532339098	-1.8852643682	-3.9565749606
H48	-0.7129983334	-2.2072418120	-3.0616796020
H49	-1.1991967116	-2.3519477389	-4.7644754518

TS6

N1	-0.1050626021	-0.1009773674	-0.0455777695
C2	-0.1126800450	-0.3841111064	2.7138624846
C3	1.0926393358	-0.1964332163	0.6292288476
C4	-1.3162978644	-0.1239771019	0.6271760749
C5	-1.3199045493	-0.2671013151	2.0064282047
C6	1.0897813189	-0.3429111404	2.0231418248
H7	-2.2686120001	-0.3003656353	2.5313186395
H8	2.0319706057	-0.4222889469	2.5548234494
N9	2.0152107125	0.0656028619	-1.5557177500
C10	4.6476124625	-0.0095406864	-0.6273401250
C11	3.0485363169	0.2073395723	-2.4019975206
C12	2.2678341763	-0.1041582772	-0.2193318332
C13	3.5909868857	-0.1485946138	0.2564544681
C14	4.3729381849	0.1785834612	-1.9905157216

H15	3.7781733498	-0.2897399738	1.3156678601
H16	5.1691591752	0.2965889281	-2.7186569349
C17	-2.1174072406	0.1547372403	-1.6539760906
C18	-4.8204202404	0.1803717053	-0.7686509210
C19	-2.4553379810	0.0279429572	-0.2721314176
C20	-3.1839611334	0.2663090729	-2.5605107083
C21	-4.5115706365	0.2845570462	-2.1298186728
C22	-3.7905261310	0.0453128542	0.1564548074
H23	-5.3147769815	0.3729500566	-2.8598226281
H24	-4.0300842220	-0.0530654791	1.2130372656
H25	-5.8559411819	0.1928205540	-0.4363155225
Ir26	-0.1287639904	0.1323946012	-1.9455252641
H27	2.7780972659	0.3459331797	-3.4431109269
H28	-2.9750331963	0.3254627497	-3.6250482218
O29	-0.1893575123	-1.7507139017	-2.5974848361
H30	-0.9123204705	-2.6527471753	-1.4919301869
O31	-0.0195793384	2.2002487493	-1.9724523758
H32	-0.9230307201	2.5102154722	-1.8253863310
C33	-0.0492094732	0.1288717208	-4.4706772304
C34	-0.6770933072	1.2727400952	-4.9847693220
C35	-0.2603018817	1.8369540825	-6.1926255757
C36	0.7889508506	1.2623753629	-6.9152543331
C37	1.4199360368	0.1159245377	-6.4245414652
C38	1.0022167704	-0.4365885912	-5.2124728036
H39	-0.4036265027	-0.7627987690	-3.6836424050
H40	-1.4723024258	1.7503769423	-4.4220897711

H41	-0.7502711843	2.7324722273	-6.5700989668
H42	1.1090872669	1.7033333521	-7.8571392917
H43	2.2311527222	-0.3426616847	-6.9873725204
H44	1.4578263288	-1.3421701035	-4.8182300810
H45	5.6722325615	-0.0441886339	-0.2663572128
H46	-0.1210337703	-0.5028063992	3.7933703716
O47	-1.1815768478	-3.1843024455	-0.6695695468
H48	-0.3618868716	-3.1612519353	-0.1611531988

TS7

Ir1	0.0210932578	-0.0242451933	0.0026541956
O2	0.0523747070	-0.0473832205	2.0435950870
C3	4.8323530821	0.1207324684	-0.6024525241
C4	3.9470628290	0.1435446509	-1.6785855800
C5	2.5738630469	0.1276989029	-1.4305032145
N6	2.1190093703	0.0835009933	-0.1514306485
C7	2.9558536134	0.0630969121	0.8878726170
C8	4.3353921830	0.0838443145	0.6999866672
H9	5.9030338515	0.1316392554	-0.7829241366
H10	4.3199836156	0.1727548461	-2.6959892775
H11	2.4582946682	0.0246925321	1.8546908632
H12	4.9996684614	0.0689940530	1.5570508806
C13	-4.3969406716	1.0857447769	-1.7549023353
C14	-3.2994198923	0.8007994969	-2.5626269596
C15	-2.0708141849	0.4339398085	-1.9941664309
C16	-1.9495304473	0.3413416405	-0.5722687181
C17	-3.0614745629	0.6465876075	0.2228171112

C18	-4.2711496033	1.0215964516	-0.3635898477
H19	-5.3428180785	1.3692322705	-2.2062391223
H20	-3.3944405293	0.8918445012	-3.6414291145
H21	-2.9675954975	0.5710215179	1.3017913142
H22	-5.1234091464	1.2554931651	0.2688814335
C23	0.6235752453	0.3880242150	-4.6893284498
C24	-0.6634146914	0.4034692829	-4.1574590897
C25	-0.8347950948	0.2976744276	-2.7717440387
N26	0.2610498080	0.1292324719	-1.9883782300
C27	1.5253704389	0.1782439212	-2.4738041850
C28	1.7343009711	0.2982578602	-3.8467608413
H29	0.7662076804	0.4705489562	-5.7622149408
H30	-1.5247998774	0.5129287126	-4.8064089852
H31	2.7380795599	0.3284132275	-4.2540752288
O32	0.2375201083	2.0328476329	0.3209851751
H33	-1.3402161642	-0.8567585962	0.1139098355
H34	0.1142570766	0.9139850433	2.1775231126
H35	-0.6294337887	2.4398575907	0.1965820201
C36	0.2711563313	-2.1381505557	-0.0221554776
C37	0.1337132986	-2.9167990994	-1.1817536152
C38	0.3775654334	-4.2940125685	-1.1629928235
C39	0.7598281866	-4.9225571630	0.0213500989
C40	0.8840237404	-4.1626172245	1.1864965865
C41	0.6351137563	-2.7885540445	1.1675091799
H42	-0.1736154457	-2.4579367091	-2.1184824716
H43	0.2632788115	-4.8738067733	-2.0767019314

H44	0.9493716030	-5.9929218210	0.0390178480
H45	1.1688143969	-4.6439209363	2.1198707390
H46	0.7074445211	-2.2014208878	2.0782108187

TS8

Ir1	0.0629963601	0.0259381859	0.0094043704
O2	0.0256230746	-0.0269632521	2.0413212173
C3	4.7897920695	0.0800542052	-0.6676217255
C4	3.8906798367	0.0288760187	-1.7280729381
C5	2.5193165430	-0.0011542738	-1.4694386082
N6	2.0674329124	0.0159672069	-0.1765458470
C7	2.9305041331	0.0647640106	0.8525700713
C8	4.3026591982	0.0967620411	0.6419515137
H9	5.8576068349	0.1072963620	-0.8605430962
H10	4.2473747559	0.0168883115	-2.7519307353
H11	2.4517226978	0.0696340970	1.8277172531
H12	4.9747610088	0.1372113229	1.4922490397
C13	-4.4855072218	0.6972318999	-1.8081158098
C14	-3.3568406144	0.4305972167	-2.5862960739
C15	-2.1658322242	0.0145483981	-1.9818914478
C16	-2.1123893101	-0.1519708220	-0.5594466795
C17	-3.2567480713	0.1467718167	0.1956432303
C18	-4.4359710048	0.5715873791	-0.4170819856
H19	-5.4015848725	1.0253574650	-2.2908891596
H20	-3.4038156274	0.5901934306	-3.6600017599
H21	-3.2096578584	0.0204495365	1.2740987791

H22	-5.3143264460	0.7988744898	0.1806701145
C23	0.5133313114	-0.2741167870	-4.6898724128
C24	-0.7651225646	-0.2475298515	-4.1280405498
C25	-0.9085493417	-0.1223763493	-2.7449518082
N26	0.2087741473	-0.0567011671	-1.9698672403
C27	1.4643224631	-0.0715790749	-2.4931815101
C28	1.6405032764	-0.1787827241	-3.8733977359
H29	0.6304065503	-0.3729954020	-5.7642999598
H30	-1.6430686838	-0.3283141882	-4.7592156991
H31	2.6353773928	-0.2008590017	-4.3033817242
O32	0.2279062116	2.0390157161	0.1551977012
H33	-1.4738300821	-1.1645323027	-0.1251653199
H34	0.0479658540	0.9149253743	2.2685073568
H35	-0.6162691291	2.4134506639	-0.1280534615
O36	-0.3671278720	-2.0548882327	0.1206911933
H37	-0.3428970988	-2.1880573812	1.0827848723

TS9

Ir1	0.0051241482	-0.0551457738	-0.0312646817
O2	-0.0317540196	-0.2624182802	2.0241497424
C3	4.7531702771	0.0759819196	-0.6731961990
C4	3.8615354077	-0.0190628833	-1.7380599868
C5	2.4892527980	-0.0450280919	-1.4851553621
N6	2.0328525857	0.0172769193	-0.1986591446
C7	2.8855649744	0.1121112323	0.8325592397
C8	4.2605014414	0.1442349344	0.6316702924
H9	5.8221419794	0.0992042691	-0.8607147123

H10	4.2252006500	-0.0660498231	-2.7582541557
H11	2.4066917245	0.1402297967	1.8068639617
H12	4.9273087402	0.2197322373	1.4835749703
C13	-4.3905235812	1.1846838463	-1.9266862522
C14	-3.3152140331	0.6846978013	-2.6594932003
C15	-2.1685065836	0.2020294343	-2.0151198982
C16	-2.1018183542	0.1834087203	-0.5806996412
C17	-3.1867867622	0.7409030444	0.1211378061
C18	-4.3139251465	1.2369996194	-0.5342246772
H19	-5.2697660151	1.5588379052	-2.4428171127
H20	-3.3518776920	0.7230972862	-3.7445772653
H21	-3.1592585523	0.7290999226	1.2068106815
H22	-5.1364172582	1.6510094247	0.0426038763
C23	0.4874723900	-0.3332642238	-4.7053829450
C24	-0.7893050367	-0.2289944020	-4.1531904610
C25	-0.9339417533	-0.0580147605	-2.7733760704
N26	0.1811428614	-0.0282821168	-1.9987175714
C27	1.4359000990	-0.1177452866	-2.5117221504
C28	1.6151126974	-0.2668128242	-3.8861587768
H29	0.6043179617	-0.4676171532	-5.7759563522
H30	-1.6659422741	-0.2841144923	-4.7880642225
H31	2.6101955236	-0.3460448839	-4.3087240587
O32	0.0318683640	1.9376164762	0.3844800534
H33	-1.8181762837	-0.8175845653	0.2484070947
H34	-0.1730045164	0.6586215963	2.2945116585
H35	-0.8184144495	2.3115738869	0.1199433136

O36	0.1007490846	-2.1558570570	-0.1895079050
H37	0.7962497960	-2.4121645933	0.4325590769
O38	-1.9886958414	-1.8514391673	1.2654822657
H39	-1.4106080139	-1.3248076077	1.8893658419
H40	-1.2697639950	-2.3378906163	0.7585291671

TS10

N1	0.0594587415	-0.1529829256	-0.0439110901
C2	0.1159170815	-0.2817458741	2.7348818151
C3	1.2407378220	-0.0643328265	0.6152861969
C4	-1.1073598647	-0.2948331068	0.6582208682
C5	-1.0889171272	-0.3792174809	2.0534258499
C6	1.2901623707	-0.1071766538	2.0094244961
H7	-2.0201899775	-0.5024450071	2.5934115681
H8	2.2536759004	-0.0035556716	2.4918120083
N9	3.3702959024	0.9951476870	0.3931632388
C10	4.0643429227	-0.4640936617	-1.8868945599
C11	4.5453180683	1.1776613602	-0.2153303772
C12	2.5179707654	0.1007569307	-0.1389748250
C13	2.8318388667	-0.6734232582	-1.2670277968
C14	4.9378393211	0.4863586468	-1.3631822720
H15	2.1395550061	-1.4333482312	-1.6222996239
H16	5.9053471625	0.6794029766	-1.8165235688
C17	-2.0839320285	-0.0769746706	-1.5577238907
C18	-4.7063349493	-0.3224891810	-0.5314231597
C19	-2.3089393264	-0.2783358342	-0.1708718058
C20	-3.1981313512	0.0164325309	-2.4058039478

C21	-4.4920303514	-0.1065203168	-1.8973601444
C22	-3.6152227438	-0.4035637248	0.3275063128
H23	-5.3403265461	-0.0325188033	-2.5732329294
H24	-3.7839343753	-0.5648172611	1.3885534093
H25	-5.7152628402	-0.4224976706	-0.1432793714
Ir26	-0.1850702256	-0.0708424941	-2.0781152872
H27	5.2082662281	1.9119247070	0.2396875147
H28	-3.0679046039	0.1935059340	-3.4696049123
O29	0.1889614526	-2.0516260471	-2.0489870659
H30	-0.1094006952	-2.4015099299	-2.9005268728
O31	-0.3354383917	0.2098989423	-4.1696797557
H32	-1.2161444692	-0.0274913377	-4.4897429514
C33	-0.1246611873	2.1637446731	-2.4485187643
C34	-1.1334997308	3.0200383612	-1.9559589183
C35	-0.8683405532	4.3534203933	-1.6455838427
C36	0.4167379909	4.8709300515	-1.8300889956
C37	1.4333028163	4.0548627310	-2.3342361791
C38	1.1604102391	2.7223148251	-2.6380231748
H39	-0.3915819121	1.3232770628	-3.4788339975
H40	-2.1373641119	2.6310622066	-1.8141317043
H41	-1.6596694236	4.9912111884	-1.2597378684
H42	0.6244499684	5.9102014056	-1.5876608342
H43	2.4310369736	4.4584719414	-2.4863745851
H44	1.9543553508	2.0960735333	-3.0411663194
H45	0.1408867933	-0.3356977957	3.8191337780
H46	4.3383458892	-1.0502651206	-2.7597542836

TS11

Ir1	0.2956723041	-0.0686564134	0.0062247384
O2	0.3778005192	-0.2679523787	1.9697782208
C3	4.9559696421	-0.0592942339	-1.2161317393
C4	3.9589204989	-0.3728097764	-2.1304497993
C5	2.6051792039	-0.2818106400	-1.7576935440
C6	2.2598869985	0.1307498909	-0.4521727045
C7	3.2753726218	0.4486583583	0.4574276420
C8	4.6124193444	0.3459970960	0.0794041269
H9	5.9999510251	-0.1279476113	-1.5073893835
H10	4.2348232037	-0.6891107320	-3.1321434145
H11	3.0246992545	0.7777650724	1.4595516820
H12	5.3925649765	0.5916573708	0.7954530911
C13	-4.3883059701	-0.9784294648	-2.0521922238
N14	-3.1432505531	-1.2829293159	-2.4311043998
C15	-2.2141441533	-0.3205515218	-2.3517766218
C16	-2.5128177483	0.9944142980	-1.9685938687
C17	-3.8171556054	1.2974983322	-1.5842707056
C18	-4.7750897943	0.2864449052	-1.6074434811
H19	-5.1151977925	-1.7859414588	-2.1139872871
H20	-4.0782523847	2.3067395248	-1.2808640862
H21	-5.8019184159	0.4736336475	-1.3094110559
C22	0.5062256009	-1.5102082058	-4.6499958008
C23	-0.7499934776	-1.2746748525	-4.0987354942
C24	-0.8517297990	-0.6902869521	-2.8365650993
N25	0.2546440921	-0.4018478225	-2.1082216340

C26	1.4927617446	-0.6188685754	-2.6431521354
C27	1.6357717653	-1.1581866626	-3.9268236656
H28	0.6001432872	-1.9560050621	-5.6355264780
H29	-1.6630883314	-1.5193041671	-4.6271154192
H30	2.6261263870	-1.3278630840	-4.3308484109
H31	-1.7488221094	1.7643467416	-1.9995508676
H32	-0.7526836115	0.9998391242	-0.4007342267
O33	-0.5630107834	-1.8349868726	0.1293747161
H34	-0.5427890813	-2.0563429065	1.0752593151
C35	0.6163928237	2.0608750257	0.1955328713
C36	0.2084031706	2.6881591849	1.3855403863
C37	0.3644151321	4.0656427163	1.5653953542
C38	0.9032816812	4.8533918299	0.5479616036
C39	1.2782921456	4.2508674335	-0.6544614427
C40	1.1355038021	2.8730197095	-0.8263316540
H41	-0.2610034433	2.1017858840	2.1706965053
H42	0.0466351514	4.5237856615	2.5005073762
H43	1.0175059948	5.9254718473	0.6849006017
H44	1.6893028699	4.8539530157	-1.4611046132
H45	1.4438587354	2.4262131111	-1.7668437170
H46	0.8876873609	0.4466597089	2.3748256135

References

[1] Sheldrick, G. M. *SHELXTL*, version 5.1; Bruker Analytical X-ray Systems, Inc.: Madison, WI, 1997.

[2] Blessing, R. H. *Acta Crystallogr.* **1995**, *A51*, 33.